Application of GC-PC-SAFT EoS to Organic Sulfur Compounds

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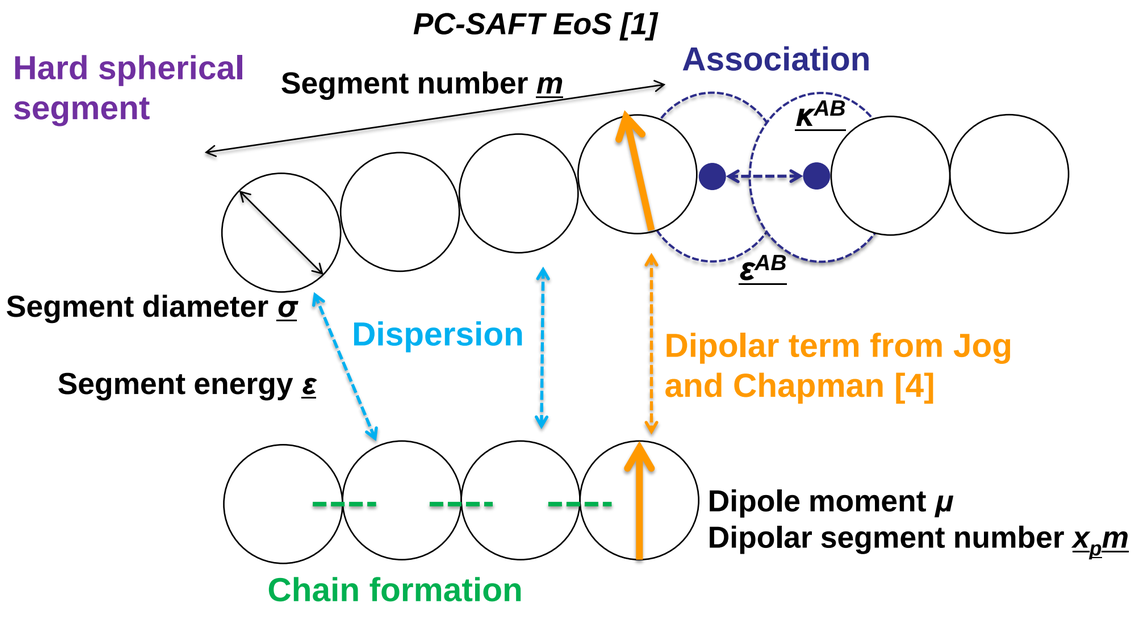
Introduction

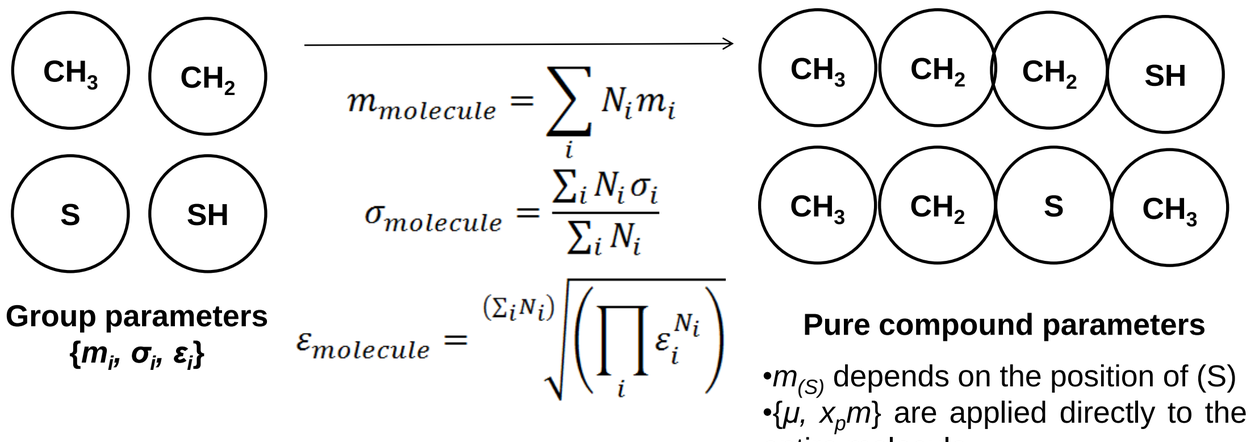
Design and optimization of separation processes require accurate knowledge of the thermodynamic properties and phase equilibria of involved pure compounds and mixtures. Thermodynamic models are thus needed to determine these properties. Model development relies on not only appropriate theory but also experimental data. However, for the organic sulfur compounds which are commonly found in diverse industrial sectors, few or even no experimental data exist in the literature. Therefore, models with predictive features may act as an alternative to handle engineering purposes.

Statistical Associating Fluid Theory (SAFT) equation of states (EoS) has been proved to be a powerful tool for modeling phase equilibria, as statistic mechanics and molecular theory were incorporated into the development. In this work, the Perturbed-Chain SAFT (PC-SAFT) EoS [1] was combined with the Group Contribution method proposed by Tamouza et al. [2]. The predictive model (named GC-PC-SAFT) was applied to investigate two series of typical organic sulfur compounds: **sulfide (R-S-R')** and **1-thiol (R-SH)**. The group parameters of (S) and (SH) were fitted to vapor pressure and liquid density data (from [3]) of 9 sulfides and 7 1-thiols, respectively. The regression results show that the average deviations on vapor pressure are generally lower than 5%, while those on liquid density are generally lower than 2%.

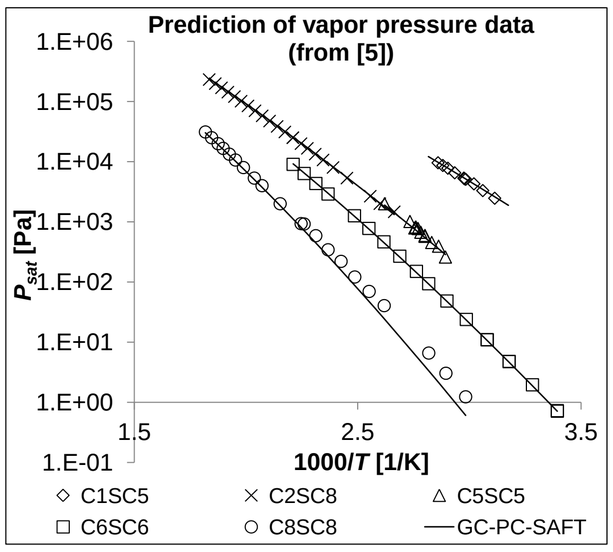
GC-PC-SAFT EoS

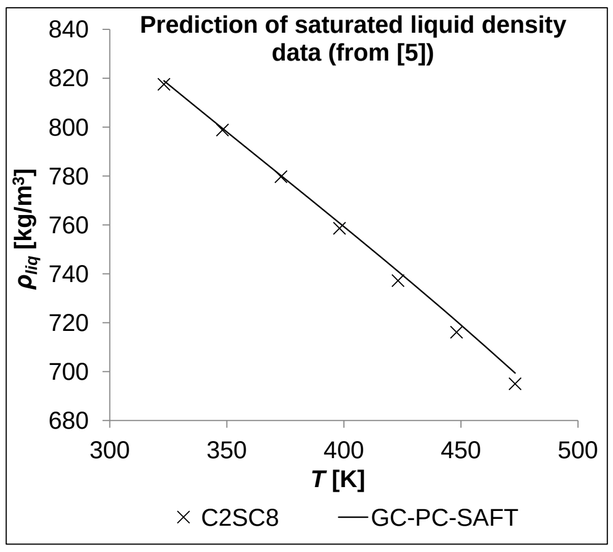


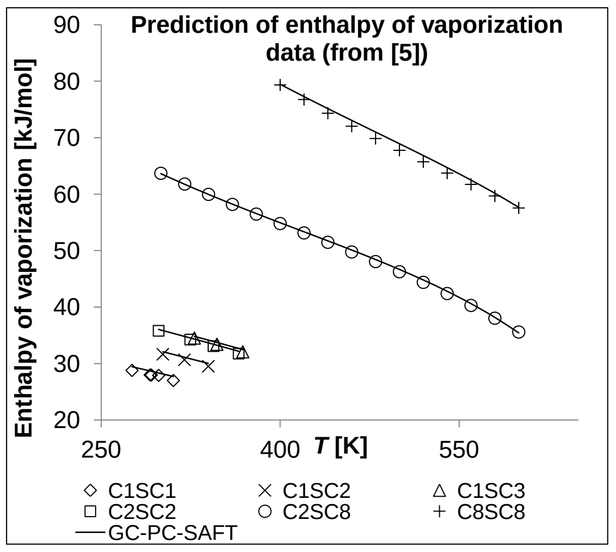
Group Contribution method of Tamouza et al. [2]

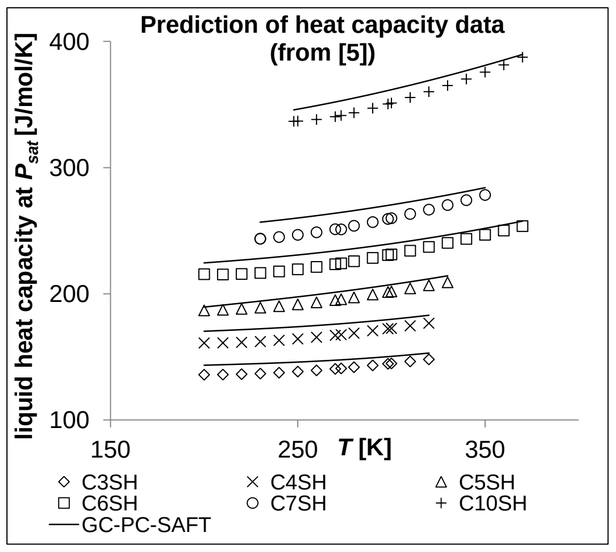


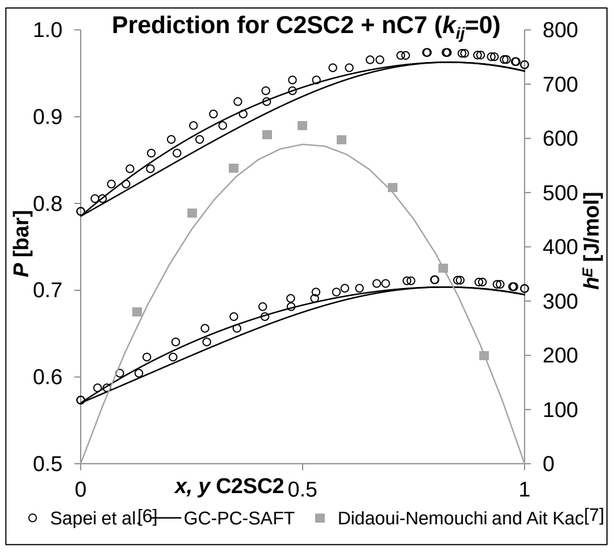
Results

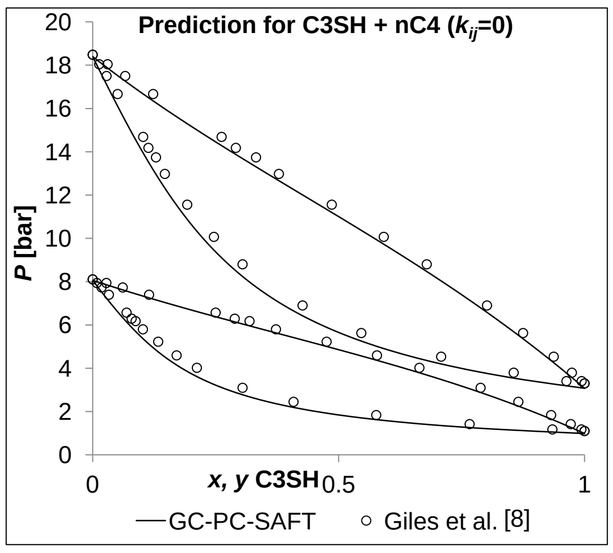


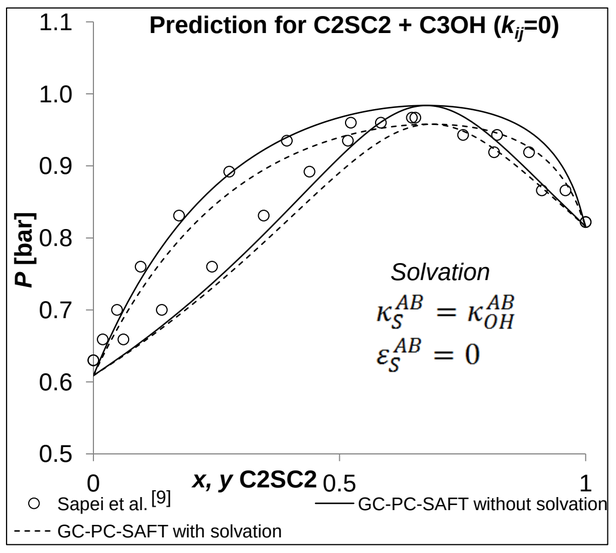


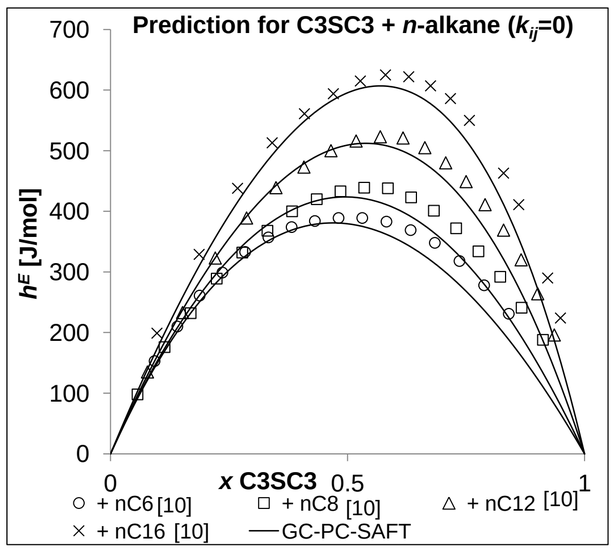












Conclusion & Perspective

✓Application of GC-PC-SAFT EoS with a dipolar term to investigate the sulfides and 1-thiols
✓Good correlation and prediction of pure compound properties (AAD generally less than 5%)
✓Satisfactory prediction of mixture VLE and h^E data without any binary interaction parameters (k_{ij}=0)

❖Prediction for multi-compound systems
❖Improvement in representing the solvation
❖Extension to other organic sulfur compounds

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